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Dynamical Initial Conditions in Quantum Cosmology

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Loop quantum cosmology is shown to provide both the dynamical law and initial conditions for the wave function of a universe by one discrete evolution equation. Accompanied by the condition that semiclassical behavior is obtained at large volume, a unique wave function is predicted.

Traditionally, physical systems are modeled mathematically by providing laws governing the dynamical behavior and specifying initial (or boundary) conditions. The latter select a particular solution to the laws, but usually all of them are allowed and describe the system under different conditions. However, in cosmology the situation is different: there is only one universe, and therefore only one fixed set of initial conditions can lead to the physically realized situation. In this context, the big bang singularity is regarded as the point of "creation" of the universe at which initial conditions (or equivalent restricting requirements) have to be imposed. Since gravity is strong at that stage and classical general relativity breaks down (signaled by the appearance of a classical singularity), a quantization of the gravitational field is needed bringing us in the realm of quantum cosmology.

The standard approach to quantum cosmology consists in quantizing a minisuperspace model which is obtained by specifying symmetry conditions, usually homogeneity and isotropy, for the allowed metrics in space-like slices of a universe. This reduces the infinitely many degrees of freedom of general relativity to finitely many ones allowing standard quantum mechanical methods [1,2]. Due to general covariance the dynamical law is provided by a constraint equation which takes the form of a second order differential equation—the Wheeler–DeWitt equation—for the wave function $\psi(a,\phi)$ depending on the scale factor $a>0$ (conventionally used as internal time) and matter degrees of freedom collectively denoted by ϕ. However, the classical singularity remains, and no initial conditions are provided by the formalism which leads at least to a two-parameter family (not counting matter degrees of freedom) of solutions and not a unique (up to norm) one. The original hopes [1] that there might be a unique solution to the constraint equation are not realized.

To address this issue, proposals have been developed by several authors. However, these proposals have considerable arbitrariness since they are driven primarily by the authors' intuition as to how the classical singularity might be smoothed out by quantum gravity. Most well-known are the "no-boundary" proposal [3] and the "tunneling" proposal [4] which both describe the "creation" of a universe at the place of the classical singularity. In all those approaches matter is regarded as being irrelevant in the early stages, and so the wave function ψ is assumed (implicitly or explicitly [5]) to be independent of the variables ϕ for small a; this is already an initial condition which strongly restricts the ϕ-dependence of ψ. We will take the same point of view concerning matter degrees of freedom here, which we regard as being justified thanks to the dominance of gravity in early stages of the evolution.

But still, there is a two-parameter family of solutions $\psi(a)$ from which one parameter has to be fixed (since the norm is irrelevant). This not only influences the wave function close to the singularity, but also its late time behavior because it selects a particular linear combination of the expanding and contracting components in a WKB-approximation. However, as an initial condition it is specified at the classical singularity (e.g., by fixing the value $\psi(0)$ [1,6] or by introducing an ad hoc "Planck potential" [5]), and thus involves Planck scale physics for which we need a full quantum theory of gravity.

One candidate for a quantization of general relativity is quantum geometry (see e.g. [7,8]) which predicts discrete eigenvalues of geometrical operators like area and volume [9–11]. A symmetry reduction [12] of the quantized (kinematical) theory to cosmological models leads to loop quantum cosmology [13], in which the discreteness of the volume is preserved [14]. All techniques used in this framework of quantum cosmology are very close to those of *full* quantum gravity, in contrast to standard quantum cosmology which is based on a *classical* symmetry reduction to a simple mechanical system and subsequent quantization. Hence, the results of loop quantum cosmology should be more reliable, in particular close to the classical singularity where the two approaches show the largest differences. In fact, loop quantum cosmology has a *discrete* evolution equation [15,16] which replaces the Wheeler–DeWitt equation and is *singularity-free* [17–19]. The fact that the Hamiltonian constraint operator of loop quantum cosmology [15] is very close to that of the full theory [20] gives rise to the hope that the results of [17] can be extended to less symmetric models.

Loop and standard quantum cosmology deviate most when applied right at the classical singularity. In this letter we will show that the particular form of the evolution equation of loop quantum cosmology, applied at vanishing scale factor, leads to a consistency condition for the

initial data. In this way the evolution equation provides both the dynamical law and initial conditions: *dynamics dictates the initial conditions*. Accompanied by a classicality condition for the solutions, a unique (up to norm) wave function is predicted.

Isotropic loop quantum cosmology. In the triad representation of isotropic loop quantum cosmology [19] the scale factor $a \in \mathbb{R}^+$ is replaced by a discrete label $n \in \mathbb{Z}$ which parameterizes eigenvalues of the triad operator. An orthonormal basis of the kinematical Hilbert space is given by quantum states $|n\rangle$ labeled by the triad eigenvalue n which also determines volume eigenvalues: $\hat{V}|n\rangle = V_{(|n|-1)/2}|n\rangle$ with

$$V_j = (\gamma l_{\rm P}^2)^{\frac{3}{2}} \sqrt{\tfrac{1}{27} j(j+\tfrac{1}{2})(j+1)} \qquad (1)$$

($\gamma \in \mathbb{R}^+$, which is of order one, is the Barbero–Immirzi parameter labeling inequivalent representations of the classical Poisson algebra, and $l_{\rm P} = \sqrt{\kappa\hbar}$ with $\kappa = 8\pi G$ is the Planck length). The volume operator has eigenvalue zero with threefold degeneracy (for the states $|\pm 1\rangle$ and $|0\rangle$), but only one of them, $|0\rangle$, has degenerate triad and so corresponds to the classically singular state. The wave function $\psi(a,\phi)$ of standard quantum cosmology is replaced by the coefficients $s_n(\phi)$ of a state $|s\rangle = \sum_n s_n|n\rangle$. For large $|n|$ the correspondence between a and n is $|n(a)| \sim 6a^2\gamma^{-1}l_{\rm P}^{-2}$ which follows from the volume spectrum ($|n| = 2j+1$).

The Hamiltonian constraint equation for spatially flat models takes the form of a discrete evolution equation (see [19] for the case of models with positive spatial curvature):

$$\begin{aligned} &\tfrac{1}{4}(1+\gamma^{-2})A_n^{(8)} s_{n+8}(\phi) - A_n^{(4)} s_{n+4}(\phi) - 2A_n^{(0)} s_n(\phi) \\ &-A_n^{(-4)} s_{n-4}(\phi) + \tfrac{1}{4}(1+\gamma^{-2})A_n^{(-8)} s_{n-8}(\phi) \\ &\quad = -\tfrac{1}{3}\gamma\kappa l_{\rm P}^2\, \hat{H}_\phi(n)\, s_n(\phi) \end{aligned} \qquad (2)$$

with

$$A_n^{(\pm 8)} := \left(V_{|n\pm 8|/2} - V_{|n\pm 8|/2-1}\right) k_{n\pm 8}^{\pm} k_{n\pm 4}^{\pm} \qquad (3)$$

$$A_n^{(\pm 4)} := \left(V_{|n\pm 4|/2} - V_{|n\pm 4|/2-1}\right) \qquad (4)$$

$$\begin{aligned} A_n^{(0)} := &\left(V_{|n|/2} - V_{|n|/2-1}\right) \\ &\times \left(\tfrac{1}{8}(1+\gamma^{-2})(k_n^- k_{n+4}^+ + k_n^+ k_{n-4}^-) - 1\right) \end{aligned} \qquad (5)$$

where V_j are the eigenvalues (1) of the volume operator with $V_{-1} = 0$, and the coefficients $k_n^{\pm}$ can be chosen to be non-vanishing by a suitable ordering of the extrinsic curvature operator and are approximately $\mathrm{sgn}(n)$ for large $|n|$ (see [19] for explicit expressions in terms of the volume eigenvalues). Here we introduced a matter Hamiltonian $\hat{H}_\phi$ whose particular form is irrelevant. It only matters that it acts diagonally in the triad degrees of freedom which is always the case in the absence of curvature couplings.

Pre-Classicality. Compared to the standard Wheeler–DeWitt equation of second order the discrete evolution equation is of order sixteen. So the problem of a unique solution seems to be more severe at first sight, but many of the additional solutions can easily be seen to not correspond to a semiclassical solution. Let us call a wave function s_n *pre-classical* if and only if, at large volume ($n \gg 1$), it is not strongly varying at the Planck scale (increasing the large label n by one), although it may oscillate on much larger scales (increasing n by a macroscopic amount). Note that a difference equation with *fixed step size*, as is always the case here, may have solutions which are very different from those of an approximating differential equation even though all solutions of the differential equation are well approximated when the step size goes to zero [21]. A common possibility is a solution with alternating sign between successive n, which cannot correspond to a continuous solution of a differential equation. Due to instabilities there can also be solutions with exponentially increasing absolute value, even in regimes where the solutions of the differential equation are purely oscillating (i.e. in the classically allowed range in a WKB approximation). A precise formulation of the phrase “not strongly varying” can be given in the following way. Note first that the Barbero–Immirzi parameter γ enters $a(n) = \gamma l_{\rm P}^2 n/6$, which is used here as internal time. Although the physical value of γ is fixed and of order one [22], we can use the $\gamma \to 0$ limit, together with $n \to \infty$ such that $a(n)$ is fixed, to decide whether a wave function is pre-classical. In this limit the difference $a(n+1) - a(n)$ becomes infinitesimal implying a continuum limit. A wave function s_n is pre-classical if and only if its limit $\gamma \to 0$, $n \to \infty$ exists, providing a rigorous check of the pre-classicality condition. Note that κ and $\hbar$, and so $l_{\rm P}$, are fixed in this limit and we are still dealing with quantum cosmology. In fact, standard quantum cosmology can be shown to be the above limit of loop quantum cosmology.

Our condition picks out only those solutions which are oscillatory on large scales but almost constant on the Planck scale. Since this is a pre-requisite for a subsequent WKB-approximation, we call it pre-classicality. Whenever it is fulfilled, a discrete wave function $s_n(\phi)$ can be approximated at large n by a standard continuous wave function $\psi(a) := s_{n(a)}$ with $n(a) = 6a^2\gamma^{-1}l_{\rm P}^{-2}$ as above, which approximately solves the standard Wheeler–DeWitt equation up to corrections of order $\sqrt{\gamma}l_{\rm P}/a$ [17,19]. Thus, standard quantum cosmology is realized only as an approximation valid at large volume where the discreteness of quantum geometry is irrelevant (see Fig. 1).

Since the Wheeler–DeWitt equation is of second order and so has two independent solutions, there can be at most two independent pre-classical solutions $s^{\pm}$ of our discrete evolution equations, such that any pre-classical

solution can be written as $s = as^+ + bs^-$ with $a, b \in \mathbb{C}$.

To demonstrate this explicitly, we introduce

$$t_m := \gamma^{-1} l_{\mathrm{P}}^{-2} (V_{2|m|} - V_{2|m|-1}) s_{4m}$$
$$P(m) := \tfrac{1}{3}\gamma\kappa l_{\mathrm{P}}^2 H_\phi(m) (V_{2|m|} - V_{2|m|-1})^{-1},$$

using the expectation value $H_\phi(n)$ of $\hat{H}_\phi(n)$ in a matter state, such that for $|n| \gg 1$, where $k_n^\pm \sim \mathrm{sgn}(n)$, the evolution equation (2) takes the form

$$\tfrac{1}{4}(1+\gamma^{-2})t_{m+2} - t_{m+1} + (\tfrac{1}{2}(3-\gamma^{-2}) + P(m))t_m$$
$$-t_{m-1} + \tfrac{1}{4}(1+\gamma^{-2})t_{m-2} = 0\,. \qquad (6)$$

In a classical regime $|m|$ is large and $P(m) \sim \frac{2}{3}\kappa H_\phi/a$ is approximately constant on a range small compared to $|m|$. In this case we have a linear difference equation with constant coefficients whose solutions can be found by an ansatz $t_m \propto e^{im\theta}$ with $\theta \in \mathbb{C}$ which in (6) yields the quadratic equation

$$(1+\gamma^{-2})\cos^2\theta - 2\cos\theta + 1 - \gamma^{-2} + P = 0$$

which has solutions

$$\cos\theta = (1+\gamma^{-2})^{-1}\left(1 \pm \sqrt{\gamma^{-4} - (1+\gamma^{-2})P}\right)$$

being real with modulus smaller than one such that θ is real when γ is of the order one and P is small.

If the matter does not contribute a Planck size energy, P is small and we have $\cos\theta_0 = 1 - \epsilon + O(\epsilon^2)$ or $\cos\theta_1 = (1+\gamma^{-2})^{-1}(1-\gamma^{-2}) + \epsilon + O(\epsilon^2)$ with $0 < \epsilon := \frac{1}{2}\gamma^2 P \ll 1$. The first possibility, expanding $\cos\theta_0 = 1 - \frac{1}{2}\theta_0^2 + O(\theta_0^4)$, leads to two solutions $\theta_0 = \gamma\sqrt{P} + O(P)$ and $-\theta_0$ with $|\theta_0| \ll 1$ both of which imply pre-classical $t_m^\pm = e^{\pm im\theta_0}$. Because γ is not large compared to one, the second possibility $\cos\theta_1$ leads to θ_1 which violates pre-classicality (e.g., for $\gamma = 1$ we have $\theta_1 = \pm\pi/2$ and $t_m \propto (\pm i)^m$).

All 16 independent solutions $t_{n/4} = \gamma^{-1} l_{\mathrm{P}}^{-2} (V_{|n|/2} - V_{|n|/2-1}) s_n$ of (2) can be obtained as

$$t_{n/4} = e^{\pm in\theta_0/4},\ e^{\pm in\theta_1/4},$$
$$(-1)^n e^{\pm in\theta_0/4},\ (-1)^n e^{\pm in\theta_1/4},$$
$$\sigma^n e^{\pm in\theta_0/4} \text{ or } \sigma^n e^{\pm in\theta_1/4}$$

where σ can be $+i$ or $-i$. Obviously, only the first two are pre-classical. The definition using $\gamma \to 0$ (a finite) is applied as follows: with $n = 6a^2\gamma^{-1} l_{\mathrm{P}}^{-2}$ we have

$$\lim_{\gamma\to 0} \gamma^{-1} l_{\mathrm{P}}^{-2} (V_{|n|/2} - V_{|n|/2-1}) = a/2\,,$$
$$\lim_{\gamma\to 0} e^{\pm in\theta_0/4} = \exp\left(\pm\tfrac{3}{2} i\sqrt{P} a^2/l_{\mathrm{P}}^2\right)\,,$$

whereas $\lim_{\gamma\to 0}\theta_1 = \pi$ and so the limit for $\gamma \to 0$, $n \to \infty$ does not exist for the remaining 14 solutions.

Thus, by using the pre-classicality requirement, which is a prerequisite for any semiclassical analysis, we arrive at the same situation as in standard quantum cosmology: there are two independent solutions from which we have to select a linear combination up to norm.

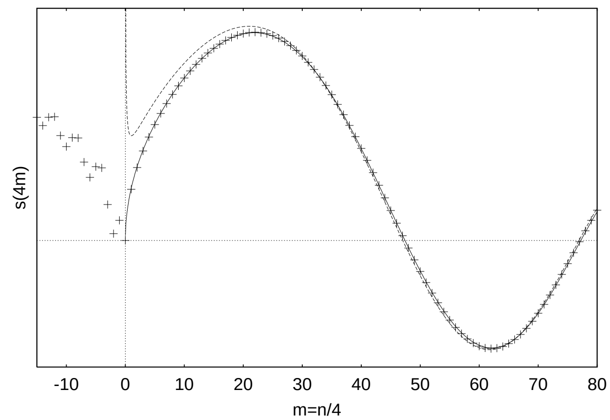

FIG. 1. The unique solution (+) of the Hamiltonian constraint (2), when the Ricci curvature is only due to a positive cosmological constant $\lambda := l_{\mathrm{P}}^2\Lambda = 2\cdot 10^{-4}$ ($\gamma = 1$), which is pre-classical for large positive n. Evolving backwards through $n = 0$, the wave function picks up a wildly oscillating component and is no longer exactly pre-classical at negative n. The standard quantum cosmology wave function $\psi(a)$, subject to $(l_{\mathrm{P}}^4(4a)^{-1}\mathrm{d}/\mathrm{d}a(a^{-1}\mathrm{d}/\mathrm{d}a) + 3\lambda a^2 l_{\mathrm{P}}^{-2})\sqrt{a}\psi(a) = 0$ in the ordering corresponding to (2), is given by $\psi(a) = a^{-\frac{1}{2}}(A\,\mathrm{Ai}(-(3\lambda)^{\frac{1}{3}}a^2 l_{\mathrm{P}}^{-2}) + B\,\mathrm{Bi}(-(3\lambda)^{\frac{1}{3}}a^2 l_{\mathrm{P}}^{-2}))$ in terms of Airy functions. Wave functions $\psi(a)$ for two choices of the parameters A and B are shown: the continuous line is the unique (up to norm) choice fulfilling DeWitt's $\psi(0) = 0$, which in this case is in good agreement with s_n at positive n, whereas any other choice leads to a diverging wave function (dashed line).

Dynamical Initial Conditions. Up to now we considered only the semiclassical regime, but there is an additional feature of loop quantum cosmology *which emerges right at the classical singularity*, deeply in the Planck regime where the approximation by standard quantum cosmology breaks down: the highest order (or lowest order when we evolve backwards) coefficient vanishes when we try to determine s_0. At first sight, it seems that this is a breakdown of the evolution similar to the classical situation. However, as demonstrated in [17,19], this is not the case in the particular factor ordering of the constraint chosen above because s_0 completely drops out of the evolution equation. (This observation depends crucially on the fact that $\hat{H}_\phi s_0(\phi) = 0$ which is always true in quantum geometry [18,19] but would be impossible without space-time discreteness.)

Instead of determining s_0 the evolution equation leads to a *consistency condition for the initial data*: starting from a general pre-classical solution $s_n = as_n^+ + bs_n^-$ for large n and evolving backwards, we eventually arrive at a

point where we have to apply (2) for $n = 8$. At this value of n the lowest order coefficient $A_8^{(-8)}$ vanishes as noted above causing s_0 to drop out. Since by assumption we have already determined all s_n for $n > 0$ (for which there is no vanishing coefficient in the evolution equation), the would-be equation for s_0 leads to a further condition for higher s_n (s_4, s_8, s_{12} and s_{16}) which upon inserting the general pre-classical solution $s_n = as_n^+ + bs_n^-$ implicitly yields a linear relation between the two free parameters a and b. *This leaves us with a unique solution* (up to norm).

Conclusions. We have shown that loop quantum cosmology implies a discrete evolution equation which uniquely determines a state (up to norm) behaving semiclassically at large volume. It is important to adapt the standard condition for semiclassicality in a WKB approximation taking the discreteness of time into account. This leads already to a strong reduction of the allowed solutions, but the crucial condition for the uniqueness arises only from the particular structure of the evolution equation in quantum geometry. We remark that in general it is only possible to require pre-classicality at one connected domain of large volume. If one evolves through a classical singularity, the wave function may pick up components which oscillate at the Planck scale (see Fig. 1). The precise form of these oscillations depends on factor ordering ambiguities (in the coefficients $k_n^\pm$ entering the constraint) and the use of the Lorentzian (versus Euclidean) theory.

Such a unique wave function generally differs from those obtained with boundary proposals of standard quantum cosmology. By choosing a real prefactor it is always real (for flat spatial slices the evolution equation has real coefficients; this no longer holds true for spatially curved models) and so cannot coincide with the "tunneling" wave function [4]. While the "no-boundary" proposal [3] also leads to a real wave function, it is imposed on the standard Wheeler–DeWitt equation at the Planck scale where large deviations to loop quantum cosmology occur. Thus, in general its wave function of a universe is different from the unique pre-classical solution found here. The consistency condition for the initial data in loop quantum cosmology may be expressed as $s_0 = 0$ which is reminiscent of DeWitt's $\psi(0) = 0$ [1] (to achieve this, an ad hoc Planck potential has been introduced in [5]). However, since these two conditions are imposed on completely different evolution equations, the selected solutions in general differ. As Fig. 1 shows, there may be a good coincidence in certain models, but only if the curvature is small at all times which can happen only in the absence of matter.

Contrary to all other proposals for boundary conditions in quantum cosmology, our *dynamical initial conditions* are not chosen to fulfill an a priori intuition about the "creation" of a universe but derived from the evolution equation which, in turn, is derived from quantum geometry, a candidate for a complete theory of quantum gravity. Therefore, one equation provides both the dynamical law and initial conditions. As we have seen, the critical condition, which crucially depends on quantum geometry, emerges from evaluating the evolution equation at the state which corresponds to the classical singularity. So in contrast to the classical situation where a singularity leads to unpredictability, in quantum geometry the regime of the classical singularity fixes ambiguities in the wave function of a universe.

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